CRS: A code to produce multigroup neutron cross sections for reactor physics calculations

Hvidtfeldt Larsen, Anne Margrethe

Publication date:
1973

Document Version
Publisher's PDF, also known as Version of record

A. E. K. Risø

Risø - M - 1568

Risø - M - 1568

Title and author(s)

CRS: A Code to Produce Multigroup Neutron Cross Sections for Reactor Physics Calculations.

by

A. M. Hvidtfeldt Larsen

Date January 1973

Department or group

Reactor Physics Department

Group's own registration number(s)

pages + tables + illustrations

Abstract

The CRS program is a multigroup cross section code, written in ALGOL for the Burroughs B6700 computer. It needs as input the so-called MASTER TAPE containing fine group cross sections and scattering matrices, and these data are in CRS made complete with thermal scattering data and shielded resonance cross sections. Spectrum calculation and condensation to fewer groups may be performed. The program has a number of output options, corresponding to different reactor physics codes in current use at Risø.

Copies to

Abstract to

Available on request from the Library of the Danish Atomic Energy Commission (Atomenergikommissionens Bibliotek), Risø, Roskilde, Denmark.
Telephone: (03) 35 51 01, ext. 334, telex: 5072.

Fi 25-204

CONTENTS

1. INTRODUCTION

The CRS (Cross Sections) program is a code to supply multigroup data for reactor physics calculations, primarily on uranium-fuelled light water reactors. It is written in ALGOL for the Burroughs B6700 computer.

A number of reports are available, describing the foundations of the program, and they should be read in connection with this report. The program needs as basic input the SIGMA MASTER TAPE the contents and formats of which are described in ref. 1. The principles of the resonance treatment are drawn up in ref. 2, and their carrying out in practice is described in ref. 3. The procedure used for generating thermal scattering data is described in ref. 4. Being a service program for the various reactor physics codes in use at Risø CRS contains several output options, matching the input of the Risø codes CELL[5], TWODIM[5], CFB[5, 6], CDB[5, 7], SYNTRON[8] and the imported codes DTF IV[9] and TWOTRAN[10].

In this report the input scheme and other information necessary to run CRS are given. In addition some description of the programming details has been included to serve as a help for the user who wants to modify the program. The present description is valid for the program version in use as at January 1st, 1973.

2. THE MAIN FEATURES OF THE PROGRAM

The basic input data for the program are the cross sections of the SIGMA MASTER TAPE[1], as mentioned in the introduction. In CRS these data are combined with resonance cross sections and thermal scattering data, collapsed to fewer groups and edited in the format needed for different reactor physics calculation codes. The flux spectrum for the condensation may be calculated at option as a 0-dimensional spectrum for the homogenized cell or by a 1-dimensional collision probability theory routine.

In the resonance region, shielded cross sections are substituted for the nuclides U^{235}, U^{238}, and Pu^{239}. For all other resonant materials the infinitely dilute cross sections from the MASTER TAPE are kept unaltered. In the case of a pin-cell calculation the resonance cross sections for U^{235}, U^{238}, and Pu^{239} may be calculated in the CRS program itself by the routine RESOREX[3] which generates the data by means of interpolation in tabulations made by the RESAB Program System[2, 11]. Otherwise these data must be calculated by RESAB directly for the problem in question.

Thermal scattering data are supplied from either NELKINSCM[4] or NELLY[12] both of which are procedures built into the CRS program. NELLY is an interpolation routine, using as input tabulations created by NELKINSCM.

It should be noted that although the program lay-out in many respects is of a very general character, the main purpose has been to supply data for light water reactors, especially the data needed for pin cell and box burn-up calculations. The production of data for other reactor configurations may well be possible, but will in many cases be more cumbersome.

3. DESCRIPTION OF THE PROGRAMMING

3.1. Program Structure

The program is built up of procedures controlled by a main program as shown in fig. 1. The lines from the main program to most of the procedures indicate that these procedures are called from the main program. To keep the program "working set" smaller than the available fast memory of the computer, the main program is made as small as possible, i.e. it contains practically nothing but the procedure calls. For the same reason, transfer of the bulk of the data from procedure to procedure is organized via files.

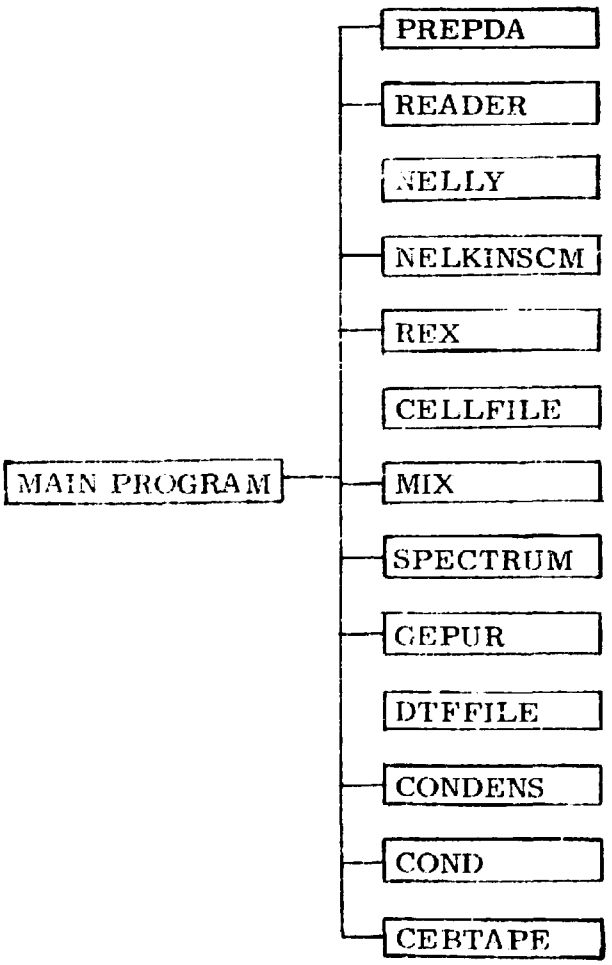

Fig. 1. CRS. Program Structure.

The procedures are declared in the main program in the sequence shown in fig. 1. Their function is as follows:

PREPDA	reads the input data blocks d-j. Prepares data for the remaining procedure calls.
READER	reads data for the materials asked for from the MASTER TAPE.
NELLY	calculates thermal scattering matrices. Called from NELKINSCM.
NELKINSCM	calculates thermal scattering matrices.
REX	calculates resonance cross sections for U^{235}, U^{238}, Pu^{239}.
CELLFILE	punches macroscopic cross sections in the format corresponding to the codes CELL and GP. Called from MIX or CONDENS.
MIX	combines the MASTER TAPE data, the thermal scattering data, and the resonance data. Calculates macroscopic cross sections for the spectrum calculation.
SPECTRUM	homogeneous spectrum calculation.
GEPUR	1-dimensional collision probability theory spectrum calculation.
DTFFILE	punches macroscopic cross sections in DTF - TWOTRAN format. Called from CONDENS.
CONDENS	calculates condensed macroscopic and microscopic cross sections.
COND	calculates and punches homogenized and/or condensed macroscopic cross sections in the TWODIM format.
CEBTAPE	prepares and punches microscopic cross sections for CEB and CDB.

3.2. Internal Files

The internal files of the program are the files used for data transfer from one procedure to another or for intermediate storing of data blocks to save fast memory space. These files are, if nothing else is mentioned, declared after the first BEGIN of the program, but in Burroughs ALGOL no reservations for a file are made before the opening of the file; i.e. a file will not

take up memory space until the first WRITE statement on it is effectuated. Immediately after the last use of each file it is removed by a CLOSE (PURGE) statement so that both the place occupied on the disc, if it is a disc file, and the buffer area in the fast memory are released.

Most of the internal files are placed on the disc (the attribute KIND is 1) for the sake of convenience. But because of the limited disc area of the computer, one of the largest files was converted into a magnetic tape file (KIND = 14). The attribute FILETYPE has been set to 6 which means that the logical record size may exceed the physical record size from the declaration (link-word files); this filetype was considered the safest in case the program should be used for different array sizes. The only exception is the file T1 which is used as a random access file and therefore has to be of the constant record length type.

The attributes MAXRECSIZE, BLOCKSIZE, AREASIZE, and AREAS have been assigned constant values corresponding to standard jobs. Special tasks may require other values which are most easily entered by a ^ FILE card in the program loader *.

In the following the name, the attributes, and the use of each internal file are given.

T1 (KIND = 1, MAXRECSIZE = 76, AREASIZE = 156, AREAS = 50):

This file is written by the procedure READER and contains the MASTER TAPE data for the materials asked for in a problem. The record numbers of the first record of each material are stored in the array PLACE which is used in procedure MIX where T1 is regarded as a random access file. Warning: This file is not a link-word file; if a problem of more than 76 groups is run, the value of MAXRECSIZE must be increased - otherwise part of the cross sections will be set to zero.

T3 (KIND = 1, FILETYPE = 6, BLOCKSIZE = 300, AREASIZE = 40, AREAS = 20):

Contains thermal scattering data. T3 is written in procedure NELKINSCM and read by procedure MIX.

T4 (KIND = 14, FILETYPE = 6, BLOCKSIZE = 77):

Magnetic tape file. Used by MIX for storing the "ready for use" 76 group microscopic cross sections. The tape is read by MIX itself when macroscopic cross sections for the compositions are prepared, and it is used again in procedure CONDENS which calculates condensed microscopic cross sections.

T5 (KIND = 1, FILETYPE = 6, BLOCKSIZE = 300, AREASIZE = 40, AREAS = 25):

*The symbol ^ is used for the invalid character of control cards

Used by MIX for intermediate storing of fission matrices to avoid the declaration of a large array holding them.

T6 (KIND = 1, FILETYPE = 6, BLOCKSIZE = 300, AREASIZE = 20, AREAS = 1):
Used in MIX to hold the scattering matrix while the mixing of fission matrices is performed.

T7 (KIND = 1, FILETYPE = 6, BLOCKSIZE = 77, AREASIZE = 155, AREAS = 1):
Transfers the macroscopic cross sections for the homogenized cell from MIX to SPECTRUM if this routine is to be used. After the reading in SPECTRUM the file is rewound and read again by CONDENS for condensation.

T8 (KIND = 1, FILETYPE = 6, BLOCKSIZE = 77, AREASIZE = 155, AREAS = 50):
Contains the condensed microscopic cross sections calculated by CONDENS. T8 is read again by the routine CEBTAPE which arranges the data in the way suitable for the codes CEB/CDB. The format of this file is very similar to that of the MASTER TAPE, and it might be used as an optional output file.

RESCS (KIND = 1, FILETYPE = 6, BLOCKSIZE = 250, AREASIZE = 1, AREAS = 10):
Used by the routine REX for the storing of the calculated resonance data which are read in MIX.

CSGP (KIND = 1, FILETYPE = 6, BLOCKSIZE = 610, AREASIZE = 10, AREAS = 10):
Transfers the macroscopic cross sections, one set for each composition, from MIX to GEPUR if the latter routine is to be used for the spectrum calculation. After that the file is rewound and saved for use in the condensation routine COND.

NELKINRES and NELLYRES, both of them declared with the same attributes, (KIND = 1, FILETYPE = 6, BLOCKSIZE = 300, AREASIZE = 10, AREAS = 50):
These two files are declared in the outer block of the procedure NELKINSCM and are used for holding the thermal scattering data from NELKINSCM itself and NELLY, respectively. At the end of NELKINSCM the data from the two files are transferred to file T3 after which the files NELKINRES and NELLYRES are purged.

3.3. Main Program

The main program of CRS has been kept as small as possible containing nothing but the necessary declarations of variables, a few READ statements,

the procedure declarations, and the statements controlling the signal flow through the procedures. After the call of each procedure the CPU-, the elapsed and the I/O-times are printed.

The input of the main program is limited to dimensioning variables and program control parameters, and the printout of these data is placed in the input routine PREPDA. The values of the four first input variables are checked as follows:

If the problem number is negative the program jumps to the label ENDOFPROGRAM. This is used after the last problem to terminate the job. The value of the day of the month must be 1-31, the month can take on values from 1-12, and the year must lie between 1969 and 1981 - otherwise the program will jump to the same label, ENDOFPROGRAM.

3.4. PREPDA

In PREPDA most of the input data are read. The first part of PREPDA is simply reading, printout of input data in the same sequence, and some checking of the input with error stops if impossible combinations of input parameters are found. In the second part PREPDA calculates data needed for the subsequent procedure calls.

3.5. READER

READER is the procedure for reading the MASTER TAPE which internally is called FILMT. Having read the first record from FILMT, the program checks the value of the variable LEG which should be 0 and that of the variable GR which should be equal to the number of groups from the input. If not, an error message is printed and the execution is stopped. The program likewise checks if all material numbers asked for are present on the tape, and stops with an error message if this is not the case.

For each new material met on the MASTER TAPE the program checks if this material is wanted for the problem. If yes, the data for the material are transferred to the disc file T1 and the corresponding element of the array MARK is set to 1. Initially all elements of MARK were set to zero. At the label CHECK it is checked whether all elements of MARK have been changed; if not, the search on the MASTER TAPE is continued.

Each time a material to be used is found, one line is printed out containing the name, number, temperature, and cell-averaged number density of the material. The record number of the first T1 record for the material is stored in the array PLACE which is used in the procedure MIX for finding the materials by random access.

3.6. NELLY

NELLY[12] calculates thermal scattering cross sections and thermal scattering matrices for the 35 lowest energy groups of the MASTER TAPE group structure given in ref. 1. The basis for the calculation is a file, internally called T100, containing the coefficients for polynomial expressions in atomic mass and temperature. T100 is included in the library at the B6700 at Risø as the data file LIBDATA/NELLY, and the connection between the two file names is obtained by a ^FILE card in the program loader.

NELLY will calculate thermal data for all materials found on the SIGMA MASTER TAPE described in ref. 1, except the materials from the fission product data file of UKNDL. These materials have the numbers from 701 to 778, and if their thermal scattering data are needed the alternative procedure NELKINSCM should be used. After the calculation NELLY prints for each material the material number, the temperature, and the name NELLY as a control. The calculated data, scattering cross sections, transport-corrected scattering cross sections, and transport-corrected transfer matrices, are stored, material by material, on the internal file NELLYRES.

The polynomial coefficients of the NELLY library file were made by least squares fitting to the thermal data in 35 groups, collapsed from 205 -group data calculated by NELKINSCM[4], a Maxwell thermal spectrum being assumed. For H and D the tables were calculated at the temperatures 293, 343, 393, 443, 493, 543, 593, and 643 K. For all other materials NELLY will interpolate between tables calculated for free atom scattering at the atomic weights 3, 6, 10, 20, 50, 100, and 250 amu and the temperatures 293, 643, 1500 and 3000 K.

3.7. NELKINSCM

NELKINSCM[4] is a procedure for calculating thermal scattering matrices. It uses the Nelkin model for H bound in H_2O and the similar model for D in D_2O, while all other materials are regarded as free atoms. The routine has been built into CRS with only slight administrative modifications. The free atom scattering cross section needed for the NELKINSCM calculation is taken as the group scattering cross section in the lowest epithermal group from the MASTER TAPE.

At the beginning of the procedure it is checked for each material if NELLY or NELKINSCM data were asked for. If NELKINSCM, the calculations are performed and a control print of the material number, of the temperature, and of the name NELKINSCM is given. The calculated data are stored on file NELKINRES. If NELLY should be used for the material, one is added to the

value of the integer variable NNELLY, the number of materials to be treated by NELLY being counted.

After the NELKINSCM calculations the arrays necessary for the call of NELLY are declared, running from one to NNELLY (if NNELLY is greater than 0). These arrays are filled by the proper values, and NELLY is then called. At last the data from the two files NELKINRES and NELLYRES are read and stored on the file T3 in the sequence expected by the procedure MIX, i.e. the sequence of the material numbers in the array NO which is determined in the data block d of the input scheme.

3.8. REX

The procedure REX is an outer block containing the connected procedures INLIB and RESOREX[3] and their calls. At first INLIB is called, reading the RESOREX library from file RESLIB which is normally the standard data file, LIBDATA/RESOREX, included in the B6700 library. After the call of INLIB, a loop is started in which the step variable TEM is running from one to NREST, the number of resonance calculations. In this loop the constants for the RESOREX call are prepared, RESOREX is called, and the results are stored on the file RESCS for later use in MIX.

For the call of RESOREX the fuel temperature is needed. In CRS, however, it is formally possible to specify different temperatures for the nuclides of the fuel mixtures. The fuel temperature for RESOREX is in PREPDA taken to be the temperature of U^{235}, U^{238} or Pu^{239}, whichever of them is met first in the input data block d. As a number density of zero is not allowed for any of the three isotopes their number densities, if zero, are put equal to 10^{-8} inside the RESOREX procedure.

After the RESOREX call, an optional calculation is inserted of correction factors to the removal cross sections of H and D in the resonance groups for the source depletion caused by resonance absorption. If it is performed, the factors are written together with the resonance cross sections on file RESCS. The correction factors are those of Askew[13]:

$$f(p) = \frac{(1-p-\chi)\ln p}{(1-p)\chi\,(1+\frac{\xi \ln p}{\tau})},$$

where p is the group resonance escape probability, ξ is the mean logarithmic decrement averaged for the cell, τ is the group lethargy width, and χ is defined as the slowing down source into the group divided by the slowing down density at the upper group boundary.

p for each of the resonance groups and ξ are calculated in RESOREX and the values of τ are read by INLIB as part of the library. χ is calculated as

$$1 - \frac{E_l}{E_u}$$

in the case of H,
and for D as

$$1 - \frac{\frac{E_l}{E_u} - \alpha + \alpha \ln \frac{\alpha E_u}{E_l}}{1 - \alpha + \alpha \ln \alpha},$$

where E_u and E_l are the upper and lower energy boundaries of the group and

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 = \frac{1}{9} \text{ for D.}$$

If the correction is ordered, the outscattering cross sections for H and D in the resonance groups will be multiplied by these correction factors in the routine MIX. The correction will be compensated in the self-scattering so that the total group scattering cross section remains unaltered.

As experience shows that the U^{238} capture resonance integral calculated from the present RESAB resonance parameter library, which is the basis of the RESOREX data, is approximately 10% too high, a correction to the U^{238} resonance capture cross sections was introduced. This correction is similar to the one reported for the code WIMS in ref. 14. If the correction is wanted, the terms

$$\Delta I_g = 0.2 \left(1 - 1.5 \frac{I_g(\sigma_p)}{\sigma_p \tau}\right) \tau \text{ barns}$$

will be subtracted from the group resonance integrals in the REG1 lowest resonance groups immediatly after the resonance integrals have been read in by INLIB (in the present library REG1 = 14). In this formula $I_g(\sigma_p)$ is the group resonance integral, τ is the lethargy width, and σ_p is the narrow resonance scattering cross section per U^{238} atom (see ref. 3).

3.9. CELLFILE

CELLFILE is a small output routine which punches macroscopic cross sections on the punch file CRSCELL in the format expected by the collision probability codes CELL[5] and GP[15]. The fission matrix is first split up into the fission spectrum and ν times the fission cross section. If punched cross sections are wanted in the group structure of the MASTER TAPE, CELLFILE is called from MIX; otherwise, if condensation is performed, the call is found in CONDENS.

3.10. MIX

At the beginning of MIX the resonance cross sections are read either from the file generated by REX or from the input cards. Then the reading of the file T1 is started parallel with the reading of the thermal data from T3.

On T1 the data of the different materials are stored in the sequence in which they were found on the MASTER TAPE. Now they are picked out by random access in the sequence determined in the input block d and scattering in the thermal groups is replaced by the thermal data of T3, which were stored by NELKINSCM in the same sequence. If the data of U^{235}, U^{238} or Pu^{239} are met, the cross sections in the resonance groups are changed for the values from input (RESAB) or RESOREX. All these modifications are followed by a corresponding change in the transport cross section. The finished fine group data are written on the internal file T4.

In the second part of MIX, macroscopic cross sections are prepared for the spectrum calculation. If the spectrum is to be calculated by GEPUR a cross section set is made for each composition, otherwise one set for the homogenized cell will be mixed. The homogenized cross section set is written on file T7 for use in SPECTRUM and CONDENS, whereas the data for GEPUR, after conversion of the fission matrix into the fission spectrum and ν times fission cross section, are stored, in the composition number order, on the file CSGP.

If RESOREX has been used for the resonance treatment two sets of resonance data are available, a fuel rod- and a cell-averaged one. Which of them is wanted in the output cross sections is specified in the input. But if SPECTRUM is to be used, the cell-averaged set is always taken for the mixture macroscopic data.

3.11. SPECTRUM

The procedure SPECTRUM calculates a homogeneous flux spectrum in the fine group structure of the MASTER TAPE. The equations for the flux

are solved directly, so only a few iterations are needed to make the eigenvalue converge. Besides the usual k_{eff} calculation, the routine is able to search criticality by varying a poison concentration or by iteration on an eigenvalue attached to an input spectrum of group-bucklings. A convergence criterion of 10^{-4} on the flux is built into the routine.

3.12. GEPUR

The procedure GEPUR is a one-dimensional (cylinder, symmetric slab, or sphere geometry) collision probability theory flux calculation routine. It is essentially the same as the program GP[15], only minor modifications have been introduced by the conversion into procedure.

GEPUR calculates the flux spectrum in the fine group MASTER TAPE structure either by k_{eff} iterations or as a source problem with an input -specified source distribution. A group-dependent buckling may be included in the calculation. The built-in convergence criterion is 10^{-5} for inner and 10^{-4} for outer iterations.

3.13. DTFFILE

For the punching of cross sections in the rather complicated format[9, 10] used for the S_n-codes, DTF IV and TWOTRAN, the small output routine DTFFILE was made. The only actions of DTFFILE are to calculate fission spectrum and ν times fission cross sections, store the cross sections in the array OUT, and punch out the fission spectrum and the OUT-array on the punched output file CRSDTF. DTFFILE is called from CONDENS after the condensation of macroscopic cross sections.

3.14. CONDENS

CONDENS is the routine which is used for condensation for all sorts of condensed cross section output except for the macroscopic TWODIM - SYNTRON output which is made by procedure COND. The cross sections prepared by CONDENS are printed out on the line printer and may in addition be edited by one of the output routines CELLFILE, DTFFILE, or CEBTAPE.

In the first part of CONDENS the macroscopic cross sections from the flux calculation are collapsed. If the spectrum is calculated by GEPUR one set is prepared for each region, otherwise only one homogenized set is made. The transport cross section is reciprocally averaged, corresponding to a flux weighting of the diffusion constant. All other cross sections are simply flux weighted.

After the condensation the conditional calls of CELLFILE and DTFFILE are inserted.

The microscopic cross sections are condensed, region by region, with the region spectrum calculated. (In the case of homogeneous spectrum calculation, all region spectra are the same). Included in the condensation for each region are all materials belonging to it, i.e. mentioned in the material list in input data block f for the composition of the region.

As in the case of macroscopic cross sections the microscopic data are directly flux weighted, except for the transport cross sections which are reciprocally weighted. The microscopic data are stored on file T8 and printed on the line printer output.

3.15 COND

COND is a routine for homogenization and condensation of the GEPUR macroscopic data. The punched output format is accepted by the codes SYNTRON[8], TWODIM[5], and CDB[7].

The condensation is the usual, diffusion constants and cross sections are flux weighted, the fission spectrum simply added for the collapsed groups. For homogenization the cross sections are weighted by flux times volume; in this case the diffusion constants are reciprocally weighted. The fission spectra are homogenized by weighting with the neutron production of the regions.

The finished cross sections from COND are punched on file FIL7.

3.16. CEBTAPE

CEBTAPE takes the microscopic data from the file T8 for editing in the format for unit cell calculations in the codes CEB[6] and CDB[7]. The punched cards for these codes contain cross sections for a fixed number of fuel isotopes and mixtures, the mixtures being the cladding material, the moderator, and two poison mixtures to be added to the fuel and the moderator, respectively.

CEBTAPE picks the fuel rod materials from region no. 1, the clad materials from region no. 2, and the moderator materials from region no. 3. (The number of regions must be 3). If a material is missing the corresponding cross sections are set to zero, and a warning is printed in the output. At last the cross sections are punched on the punch file RSCEB and written on the line printer for control.

4. INSTRUCTIONS FOR RUNNING THE PROGRAM

4.1. Material Numbers and Standard Parameter Values

The materials for which cross sections are produced are identified by tneir material numbers. The numbers for the materials available from the SIGMA MASTER TAPE are given in ref. 1, and both the identifier NO of input data block d and the arrays REGM and REGM 1 of input data block f refer to these numbers. In some cases materials which are not found on the SIGMA MASTER TAPE are important; if group data sets for such materials have been procured, a program[16] exists which will edit them on a new tape in the MASTER TAPE format together with the data of the selected materials from the SIGMA MASTER TAPE. This new MASTER TAPE can then be used with the CRS program.

Although most of the array dimensioning parameters are variable and specified by input, some of them are in practice fixed on account of the standard libraries. The number of groups on the SIGMA MASTER TAPE is 76, and if this library is to be used the number of fine groups in CRS must be the same. The number of thermal groups is free if NELKINSCM is used for the thermal data, but if NELLY is wanted 35 thermal groups have to be specified. For the resonance treatment the number of resonance groups for U^{238}, REG, and for U^{235} and Pu^{239}, REG 1, must be specified. If RESOREX is to be used with its standard library the values are REG = 22 and REG 1 = 14.

4.2. Restrictions

A number of more or less intentional restrictions exists in the CRS program. The reasons for these restrictions are not all obvious, but so far they have not been sufficiently inconvenient to justify the investment of the programming work which is required to remove them. The most important ones are given here.

If one of the routines RESOREX and/or CEBTAPE is used the cell specified must be a 3-region cylindrical pin cell in which region number one is the fuel, region number 2 the clad, and region number 3 the moderator. CEBTAPE will not accept a value of the parameter NREST different from one. The number of temperatures specified for the three resonance isotopes U^{235}, U^{238}, and Pu^{239} must be equal to the value of NREST, and the fuel temperatures for the RESOREX calculation will be the temperatures of the first of the three nuclides met with in the input block d.

The number of resonance groups is given as the input variables REG and REG 1, but the lowest resonance group is bound to be the first group above

the thermal groups. Expressed by the variable names from the input scheme, the resonance region of U^{238} is the groups from GRP - NTHG - REG + 1 until GRP - NTHG, and analogously for U^{235} and Pu^{239}.

The thermal data of the NELLY routine are identified by the MASTER TAPE identification numbers, and all materials from the SIGMA MASTER TAPE except the fission products, 701-778, are known by NELLY. For the materials numbers 701-778 and for "foreign" materials, NELKINSCM has to be used.

The use of the condensation and homogenization routine COND requires that the spectrum should be calculated by GEPUR.

4.3. Program Loader

The CRS program is included in the monthly updated library at the B6700 installation of Risø. Normally the source form of the program is used so that modifications are possible. A printout of the loader is shown in fig. 2. The invalid character in column 1 of control cards is represented by a ^.

The program file name (SOURCE/CRS) may be changed if program modifications are introduced, and consequently the ^ ALGOL FILE card must be updated. At present (January 1973) the latest updated program version is called SOURCE/CRSDEC.

Correction cards may be inserted between the $ RESET LIST card and the ^ DATA RSCCR card. The card input data must follow after the ^ DATA RSCCR.

```
^COMPILE CRS          ALGOL          !PROCESS     300, 20001,AML
^ALGOL FILE TAPE = SOURCE/CRS
^FILE FILMT=AEK134
^FILE RESLIB=LIBDATA/RESOREX
^FILE T100=LIBDATA/NELLY
^DATA
$SET MERGE
$RESET LIST


^DATA RSCCR


^  END OF JOB 3 6700
```

Fig. 2. CRS Loader

4.4. Job Request Card

It is important to give the operator instructions of necessary tape mounting. This is done by filling out the so-called "job request card". Here the maximum elapsed time, the number of punched cards, the magnetic tapes to be mounted, and the library files to be used must be given.

For a standard job the tapes are:

1. The MASTER TAPE for which the appropriate AEK-number must be given
2. One scratch tape

The library files then are:

1. The program file SOURCE/CRS
2. The data file LIBDATA/RESOREX (if RESOREX is used)
3. The data file LIBDATA/NELLY (if NELLY is used)

In special cases the library data files may be converted into input tapes by a ^FILE card.

4.5. Computing Time

The computing time for a job with few regions in the flux calculation is about 1 minute elapsed per material plus punching time if punched cards are produced. If more than 3 compositions are specified, the flux calculation, however, becomes very time-consuming, and computing time will increase rapidly with the number of compositions and regions. The elapsed time for each of the two jobs used as examples in this report was approximately 20 minutes.

5. INPUT

5.1. Input Files

The CRS input files are the following:

FILMT = the MASTER TAPE input file. Must be AEK 42, AEK134, or another tape in the MASTER TAPE format. The connection between the internal file name FILMT and the actual tape is obtained by a ^ FILE card in the program loader.

RESLIB = the RESOREX library. Only necessary if RESOREX is used. The standard RESOREX library LIBDATA/RESOREX may be called in by a ^FILE card.

T 100 = the NELLY library. Only necessary if NELLY is used. The standard NELLY library LIBDATA/NELLY may be called in by a ^ FILE card.

RSCCR = the card input file. The contents of this file are described in the input scheme given below.

5.2. Input Scheme

In the input scheme the input quantities are called by their variable names and the type of variable is given by the abbreviations:

I integer
IA integer array
R real
RA real array
AA alpha array

In Burroughs ALGOL every logical record (read statement) must begin on a new card. The card shifts made necessary for this reason are indicated by a horizontal line between the variable names. Where no format is specified the data are read in free field format.

a) Heading data.

SYMBOL	FORMAT	TYPE	DIMENSION	SPECIFICATION
HEADTEXT	12A6	AA	[1:12]	72 columns problem description. Appears in the heading of each page of output
PROBNO		I		Problem number
DAY		I		Day of the month
MONTH		I		Month
YEAR		I		Year

b) Dimensioning variables and program control parameters.

SYMBOL	TYPE	SPECIFICATION
COMP	I	Number of materials to be read from the MASTER TAPE
GRP	I	Number of energy groups on the MASTER TAPE
NTHG	I	Number of thermal groups
NTEMPMAX	I	Maximum number of temperatures for a material
NREST	I	Number of resonance calculation sets
GEOM	I	Geometry indicator 1: cylinder 2: slab 3: sphere
NC	I	Number of compositions
NR	I	Number of regions
CG	I	Number of condensed energy groups (redundant if RED = 5)
RES12	I	Resonance calculation indicator 0: none of the isotopes U^{235}, U^{238}, Pu^{239} occurs in this problem 1: resonance data are supplied as input 2: resonance calculation will be performed by RESOREX
SPEC	I	Spectrum calculation indicator 0: spectrum not calculated 1: homogeneous spectrum calculation by the routine SPECTRUM

SYMBOL	TYPE	SPECIFICATION
		2: 1-dimensional spectrum calculation by the collision probability routine GEPUR 3: 1-dimensional GEPUR spectrum calculation where one or more unit cell regions are homogenized
KRI	I	If SPEC = 0: redundant If SPEC = 1: KRI = 1: k_{eff} calculation KRI = 2: critical poison calculation KRI = 3: critical buckling calculation If SPEC = 2 or 3: KRI = 1: k_{eff} calculation KRI = 2: source problem
RED	I	Cutput parameter -1: no condensed cross sections 0: condensed microscopic and macroscopic cross sections are printed, but no punched output 1: microscopic cross sections for the codes CEB and CDB are punched 2: macroscopic cross sections for the codes GP and CELL are punched. If SPEC = 0 or 1, one homogenized set, otherwise one for each region 3: macroscopic cross sections for DTF or TWOTRAN are punched. If SPEC = 0 or 1, one homogenized set, otherwise one for each region 4: no condensed cross sections. Fine group macroscopic cross sections are punched for GP or CELL. (SPEC should be set to 0) 5: macroscopic cross sections, condensed and/or homogenized, for the programs TWODIM, CDB, and SYNTRON are punched

c) Number of materials in the compositions.

SYMBOL	TYPE	DIMENSION	CONDITION	SPECIFICATION
NM	IA	[1:NC]		Number of materials in each composition. If a material occurs with more than one temperature in a composition, the different temperatures are counted as different materials. In the case of a fuel region to be homogenized (SPEC = 3) the corresponding element of NM is the sum of the elements in the array NM 1, giving number of materials for the regions of the sub-cell
NBP	I		RED=1	Number of materials in the mixture used as burnable poison in the fuel rod in CEB or CDB
NPOI	I		RED = 1	Number of materials in the mixture used as moderator poison in CEB or CDB

d) Material list. Data block d is repeated COMP times.

SYMBOL	TYPE	REPETITION	SPECIFICATION
NO	I		Material identification number
NTEMP	I		Number of temperatures for this material
THERSC	I	xNTEMP	Thermal scattering indicator 0: No thermal scattering matrix 1: Thermal scattering data for this material calculated by NELKINSCM 2: Thermal scattering data for this material calculated by NELLY 3: Thermal scattering data for this material is supplied as input
TEMP	R		Temperature (degrees absolute)

e) Cell dimensions and distribution of compositions.

SYMBOL	TYPE	DIMENSION	SPECIFICATION
R	RA	[0:NR]	Radii or x-values of the regions (cm)
CPN	IA	[1:NR]	Composition numbers of the regions

f) Description of compositions. Data block f is given for each composition, i.e. NC times.

SYMBOL	TYPE	DIMENSION	CONDITION	REP-ETITION	SPECIFICATION
I	I				Composition number. A negative value of I indicates that region no. ABS(I) is a fuel region to be homogenized (SPEC=3)
REGM	IA	[1:NM[I]]			Material numbers in this composition
REGT	IA	[1:NM[I]]	I> 0		Corresponding temperature numbers (referring to the sequence in data block d)
REGD	RA	[1:NM[I]]			Corresponding number densities in units of 10^{24}
GEOM 1	I				Geometry indicator for sub-cell. 1: cylinder 2: slab 3: sphere
NC 1	I				Number of compositions in sub-cell
NM 1	IA	[1:NC1]	I< 0		Number of materials in each composition of sub-cell

SYMBOL	TYPE	DIMENSION	CONDITION	REPETITION	SPECIFICATION
R 1	RA	[0:NC1]			Radii or x-coordinates of sub-cell(cm)
I 1	I				Sub-composition number
REGM 1	IA	[1:NM1 [I1]]			Material numbers in sub-composition no. I1
REGT 1	IA	[1:NM1 [I1]]		xNC1	Corresponding temperature numbers
REGD 1	RA	[1:NM1 [I1]]			Corresponding number densities in units of 10^{24}

g) Resonance data.

SYMBOL	TYPE	SPECIFICATION
AVE	I	1: Resonance cross sections are fuel-averaged 2: Resonance cross sections are cell-averaged
REG	I	Number of U^{238} resonance groups
REG 1	I	Number of U^{235} and Pu^{239} resonance groups. If RES12= 1 REG must be greater than REG 1. If RES12= 2 the values of REG and REG1 must correspond to the RESOREX library values
CORU238	I	Indicator for correction to U^{238} cross sections 1: correction 0: no correction
CORHD	I	Indicator for resonance correction to H and D removals 1: correction 2: no correction

h) Data for flux calculation.

SYMBOL	TYPE	DIMENSION	CONDITION	REPE-TITION	SPECIFICATION
FL	RA	[1:GRP]	SPEC=0 ∧RED≠4		Group fluxes for cross section condensation
NOBU	I				Number of different group bucklings
CMG	I				"Coarse mesh groups", number of buckling mesh
BUCKNO	IA	[1:CMG]	SPEC≠0 ∧RED≠4		Number of energy groups in each mesh (higher energy mesh first)
SAM	IA	[1:CMG]			Buckling number in each mesh (highest energy mesh first)
BUCKIN	RA	[1:NOBU]			Values of buckling (cm^{-2})
CONTR	RA	[1:GRP]	SPEC=1 ∧KRI=2 ∧RED≠4		Poisoning cross section. The concentration of this material will be varied until criticality is obtained
SD	RA	[1:GRP]	SPEC=2or3 ∧KRI=2 ∧RED≠4	xNR	Source distribution in the regions from 1 to NR
A	R		SPEC= 2 or 3 ∧RED≠4		If ≥0: greyness in all groups 0: black, 1: white
GR	RA	[1:GRP]	A<0		Greyness array
U	I				Composition number for a composition containing fuel. The fission spectrum for the flux calculation is taken from this composition

i) Condensed group structure.

SYMBOL	TYPE	CONDITION	REPETITION	SPECIFICATION
GMAX	I	RED≠4 RED≠5	xCG	Upper and lower fine groups in the condensed group structure, starting at the highest energy group
GLOW	I			

j) Poison compositions for CEB-CDB output.

SYMBOL	TYPE	DIMENSION	CONDITION	SPECIFICATION
INPOI	IA	[1:NPOI]		Material numbers for materials in moderator poison
DPOI	RA	[1:NPOI]		Corresponding densities
INBP	IA	[1:NBP]	RED=1	Material numbers for materials in burnable poison of fuel rods
DBP	RA	[1:NBP]		Corresponding densities

k) Thermal scattering data block.

SYMBOL	FOR-MAT	TYPE	DIMENSION	CONDITION	REPE-TITION	SPECIFICATION
SS	6E12.5	RA	[1:NTHG]	THERSC=3 for one or more materials	for each material having THERSC=3	Thermal scattering cross section
ST		RA	[1:NTHG]			Transport-corrected scattering cross section
SCM		RA	[1:NTHG, 1:NTHG]			Thermal transfer matrix. The sequence of materials must be that of data block d

l) RESAB-cards. Only if RES!2=1.
Repeated NREST times.

1) A set of heterogeneous RESAB FILE 1 punched cards in REG 1 groups for the three resonance nuclides in the sequence U^{238}, U^{235}, Pu^{239}.
2) A set of homogeneous RESAB FILE 1 punched cards in REG-REG 1 groups for U^{238}.
The formats are described in ref. !1 pp. 46-47.

m) Input for homogenization and/or condensation of macroscopic TWODIM/SYNTRON cross sections.
Repeated until CON = 0 is read.

SYMBOL	TYPE	DIMENSION	CONDITION	REPE-TITION	SPECIFICATION
CON	I				If CON=0 no further homogenization and/or condensation is performed. If homogenization and/or condensation is wanted, CON=1
NCE	I				Number of regions to be homogenized
NCG	I		RED= 5		Number of condensed energy groups
REGC	IA	[1:NCE]			The numbers of the regions to be homogenized
GMAX	I				Upper and lower fine groups
GLOW	I			xNCG	in the condensed group structure, starting at the highest energy group

a) After the last problem

PUNCH	SPECIFICATION
FF	Text-card
-1	Negative problem number terminates the job

6. OUTPUT

6.1. Printed Output

The first part of the printed output from CRS is a printout of the input data blocks b - j. After each procedure the process, the elapsed, and the I/O times are printed.

The number densities printed from the procedure READER are the cell averaged for each material. If condensation is performed the condensed cross sections are printed, and the different cross section types are characterized by their PCN's from the MASTER TAPE[1]. If punched output is ordered, the line printer output will contain a copy of the punched cards.

6.2. Punched Output

The present version of the program has four options for punched output:

1) If the parameter RED in input data block b is 1 the program will produce punched microscopic cross sections in the format needed for CEB[6] or CDB[7]. The number of compositions and regions, NC and NR from data block b, should both be equal to 3 if this sort of output is wanted, and the program will take regions nos. 1, 2, and 3 as the fuel, clad, and moderator region respectively.

   The materials for which cross sections are punched are the following:

   Burnable poison, U^{235}, U^{236}, U^{238}, Pu^{239}, Pu^{240}, Pu^{241}, Pu^{242}, Xe, Sm, FP, and O condensed with the spectrum calculated for region no. 1.

   Cladding material condensed with the spectrum calculated for region no. 2.

   Moderator material and moderator poison condensed with the spectrum calculated for region no. 3.

   The cross sections for a mixture are average microscopic cross sections, and the corresponding number density is the sum of the number densities of the components.

   A material to be punched should be present in the region to which it belongs, i.e. specified with corresponding number density in the data block f of the input scheme. Otherwise the program will put all cross sections of the missing material to zero and write an error message in front of the listing of the punched cards. If a material is wanted in the output without contribution to the calculated spectrum it must be included in the composition with a corresponding number

density of zero. The punch file for this output is called RSCEB.

The input for a run producing CEB-CDB cross sections is shown as input example no. 1.

2) If RED is 2 or 4 macroscopic cross sections in CELL[5] format will be punched. For RED = 2, one set of condensed cross sections is punched for each region (NR cross section sets if SPEC = 2 or 3, only one if SPEC = 1).

In the case of RED = 4, the parameter SPEC should be 0 and one set of cross sections will be punched for the homogenized cell in the fine group structure of the MASTER TAPE.

The cross sections of this format are:

fission spectrum
absorption cross section (capture + fission)
scattering matrix
fission cross section
ν times fission cross section

The punch file for CELL output is called CRSCELL.

3) If RED is 3, the program will punch NR sets of macroscopic cross sections in the format needed for the S_n-codes DTF IV and TWOTRAN, one set for each region. (In the case of SPEC = 1, only one set is produced). The format is described in ref. 9. This punch file is called CRSDTF.

4) If RED is set to 5, homogenized and/or condensed macroscopic cross sections may be produced in the format corresponding to the input of TWODIM,[5] SYNTRON[8] and non-burnable regions in CDB[7]. This output option requires a spectrum calculated by GEPUR, i.e. SPEC = 2 or 3. The parameter KRI should be 1, otherwise only diffusion constant and scattering matrix are punched.

The cross sections are:

diffusion constant

scattering matrix, diagonal elements are replaced by removal plus absorption cross section

fission spectrum

ν times fission cross section

fission cross section

The punch file name for this output is FIL 7. Test example no. 2 is a run producing TWODIM cross sections.

7. INPUT EXAMPLES

7.1. Example No. 1

Microscopic cross sections punched for CEB/CDB

```
  TEST CRS        DRESDEN1 PIN 50% VOID 0 MWD/TU FUEL TEMP 1273 DEG K
1,
19,12,1972,
14,76,35,2,1,1,3,3,10,
2,1,1,1,
11,2,3,
1,1,
5,1,
2,1273,
7,1,
2,1273,
31,2,
2,1273,
2,557,
36,1,
2,567,
37,1,
2,567,
41,1,
2,557,
6,1,
2,1273,
9,1,
2,1273,
10,1,
2,1273,
11,1,
2,1273,
28,1,
2,1273,
19,1,
2,1273,
15,1,
2,1273,
50,2,
2,1273,
2,557,
0,0.6323,0.7252,1.0193,
1,2,3,
1,
5,7,31,9,10,11,6,15,19,28,50,
1,1,1,1,1,1,1,1,1,1,1,
3.460E-4,2.242E-2,4.554E-2,0,0,0,0,0,0,0,0,
2,
36,37,
1,1,
3.55E-2,7.57E-5,
3,
41,31,50,
1,2,2,
2.49E-2,1.245E-2,0,
```

To be continued

Continuation (example 1)

```
1,22,14,
1,0,
1,1,
76,1,3.3E-4,
1,13,
14,26,
27,30,
31,41,
42,47,
48,52,
53,55,
56,63,
64,70,
71,76,
50,1,50,1,
FF
-1
```

7.2. Example No. 2

Macroscopic cross sections punched for SYNTRON/TWODIM

```
 WATER GAP CROSS SECTIONS   DRESDEN I
1,
29,9,1972,
12,76,35,2,1,2,3,8,5,
2,3,1,5,
2,4,13,
5,1,
2,814,
7,1,
2,814,
31,2,
2,814,
2,557,
36,2,
2,567,
2,557,
37,2,
2,567,
2,557,
41,1,
2,557,
6,1,
2,814,
9,1,
2,814,
10,1,
2,814,
11,1,
2,814,
19,1,
2,814,
15,1,
2,814,
0,0.2576,0.5156,0.9061,1.506,2.306,3.306,4.806,6.306,
1,1,2,3,3,3,3,3,
1,
31,41,
2,1,
2.4880E-2,4.9760E-2,
2,
41,31,36,37,
1,2,2,2,
2.91509E-2,1.45754E-2,1.66645E-2,3.55145E-5,
```

To be continued

Continuation (example 2)

```
-3,
1,3,
9,2,2,
0,0.63,0.7252,1.0193,
1,
5,7,31,9,10,11,6,15,19,
1,1,1,1,1,1,1,1,1,
3.266E-4,2.265E-2,4.604E-2,2.033E-5,7.498E-7,7.650E-8,4.340E-6,
3.821E-6,3.797E-9,
2,
36,37,
1,1,
3.470E-2,7.400E-5,
3,
41,31,
1,2,
3.736E-2,1.868E-2,
2,22,14,
1,0,
1,1,
76,1,0,
1,
3,
1,
2,5,
1,2,
1,13,
14,26,
27,41,
42,55,
56,76,
1,
1,5,
3,
1,13,
14,26,
27,41,
42,55,
56,76,
0,
FF
-1,
```

8. REFERENCES

1) A.M. Hvidtfeldt Larsen, SIGMA MASTER TAPE, a Multi-Group Cross Section Library. Risø Report No. 262 (1972) 50 pp.

2) J. Mikkelsen, The Neutron Resonance Reactions in Thermal Nuclear Reactors Determined by Semi-Analytic as well as Numerical Methods. Risø Report No. 234 (1970) 167 pp.

3) H. Neltrup, RESOREX, a Procedure for Calculating Resonance Group Cross Sections. Risø-M-1437(1971) 25 pp.

4) C.F. Højerup, Om procedure NELKINSCM til beregning af termiske spredningsdata. Risø-M-1379 (in Danish, 1971)(Internal Report) 11 pp.

5) K.E. Lindstrøm Jensen, Development and Verification of Nuclear Calculation Methods for Light-Water Reactors. Risø Report No. 235 (1970) 161 pp.

6) L. Mortensen, The Fission Product Treatment in the CEB Unit Cell Burnup Programme. Risø-M-1356 (1971) 69 pp.

7) C.F. Højerup. User's Manual for the Programme CDB 2 as of October 1st, 1972. Risø-M-1546 (Internal Report) (1972) 21 pp.

8) H. Larsen, SYNTRON, a Three-dimensional Flux Synthesis Programme. Risø-M-1346 (1971) 33 pp.

9) K.D. Lathrop, DTF 4, A FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering. LA-3373 (1965). 141 pp.

10) K.D. Lathrop, User's Guide for the TWOTRAN (x, y) Program. LA-4058 (1968) 23 pp.

11) J. Mikkelsen and P. Kirkegaard, A User's Guide to the RESAB Program System for the B 6700 Computer. Risø-M-1477 (1972) 53 pp.

12) C.F. Højerup, Risø, Denmark, unpublished work (1972).

13) J.R. Askew, The Calculation of Resonance Captures in a Few-Group Approximation. AEEW-R 489 (1966) 23 pp.

14) F.J. Fayers, P.B. Kemshell and M.J. Terry, An Evaluation of some Uncertainties in the Comparison between Theory and Experiment for Regular Light Water Lattices.
J. Brit. Nucl. Energy Soc. 6 (1967) p. 166.

15) C.F. Højerup, Risø, Denmark, unpublished work.

16) L. Mortensen, Risø, Denmark, personal communication (1973).